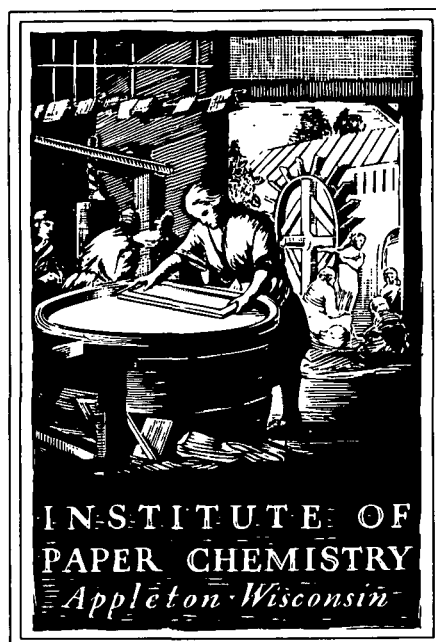


PROJECT ADVISORY COMMITTEE

Subcommittee on
Systems Analysis



IPC STAFF STATUS REPORTS

This information represents a review of on-going research for use by the Project Advisory Subcommittees. The information is not intended to be a definitive progress report on any of the projects and should not be cited or referenced in any paper or correspondence external to your company.

Your advice and suggestions on any of the projects will be most welcome.

FOR MEMBER COMPANIES ONLY

NOTICE & DISCLAIMER

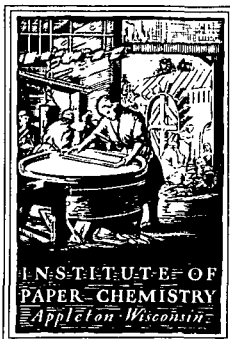
The Institute of Paper Chemistry (IPC) has provided a high standard of professional service and has exerted its best efforts within the time and funds available for this project. The information and conclusions are advisory and are intended only for the internal use by any company who may receive this report. Each company must decide for itself the best approach to solving any problems it may have and how, or whether, this reported information should be considered in its approach.

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THE INSTITUTE OF PAPER CHEMISTRY

Post Office Box 1039
Appleton, Wisconsin 54912
Phone: 414/734-9251
Telex: 469289

October 5, 1987

TO: Members of the Systems Analysis Project Advisory Committee

Enclosed is advance reading material for the October 27-28 meeting of the Systems Analysis Project Advisory Committee. Included is a status report, an agenda, and a current committee membership list.

The development of a "user friendly" interface for the μ MAPPs editor and the extension of performance attribute prediction to the kraft process have been the focus of our efforts during the last reporting period. The performance modeling work is summarized in this report; the user interface will be demonstrated at the meeting.

The MAPPs Users Group has been invited to attend the Tuesday afternoon session of the PAC meeting, and will be holding their formal meeting Tuesday evening and Wednesday morning. The MUG and the PAC provide timely and important input to the development of MAPPs. Please try to attend the meeting, but if you cannot, please send me your comments and thoughts on the future needs and directions for MAPPs.

Rooms have been reserved in the Continuing Education Center, and meals will be provided as stated on the agenda. If you haven't already indicated your attendance, please do so at your earliest convenience by returning your registration form or calling Sandy Berghuis at 414/738-3202.

For all Project Advisory Committee meetings, the Institute invites its member companies to send one or more representatives to attend the review sessions (first day) of any or all of the meetings. These invitations were mailed September 1. PAC members from member companies are also welcome to attend the other meetings, and may stay in the CEC and attend meetings and meals of their choice, at no cost. If you wish to attend any of the other meetings, but haven't registered, please call Sandy Berghuis to do so. A meeting schedule is enclosed for your information.

We look forward to meeting with you on October 27-28.

Sincerely,

Clyde H. Sprague, Director
Engineering Division

CHS/lis
Enclosures

1043 East South River Street

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PRELIMINARY AGENDA
SYSTEMS ANALYSIS PROJECT ADVISORY COMMITTEE*

October 27-28, 1987

Continuing Education Center (CEC)
The Institute of Paper Chemistry
Appleton, Wisconsin

Tuesday, October 27, 1987

12:00 - 1:00	Lunch	
1:00 - 1:15	Introductory Remarks	Clyde Sprague
1:15 - 1:45	MAPPS Status Review	Pete Parker
1:45 - 2:30	The User Friendly Interface	Mike Schreiter
2:30 - 5:00	Performance Attribute Modelling	Gary Jones Pete Parker
5:30 - 6:00	Cocktails	
6:00	Dinner	

Wednesday, October 28, 1987⁺

7:30	Breakfast	
8:30 - 9:30	Review of Strategic Research Plan	Ron Yeske Clyde Sprague
9:30 - 11:00	Committee Planning Session	

* The MAPPS Users Group will be meeting with the PAC on Tuesday afternoon

+ Program Advisory Committee members only

NOTE: The spring Systems Analysis PAC meeting is scheduled for March 29-30, 1988.

SYSTEMS ANALYSIS

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*date of retirement
10/5/87
ls

THE INSTITUTE OF PAPER CHEMISTRY

Appleton, Wisconsin

Status Report

to the

SYSTEMS ANALYSIS

PROJECT ADVISORY COMMITTEE

Project 3471

PROCESS MODELING AND SIMULATION

September 25, 1987

PROJECT SUMMARY FORM

DATE: October 1, 1987

PROJECT NO. 3471 - Process Modeling and Simulation

PROJECT LEADER: P. Parker

IPC GOAL:

To develop and support the simulation capabilities required by our member companies.

OBJECTIVE:

To develop and support the MAPPS simulation package.

CURRENT FISCAL YEAR BUDGET: \$150,000

SUMMARY OF RESULTS SINCE LAST REPORT: (February, 1987 - September, 1987)

Version 3.0 was released in late March and has been well received by our clients.

We have made our first non-U.S. sale and are in the process of establishing a marketing arrangement with a consultant to supply the South American market with MAPPS.

A "user friendly" interface for the μ MAPPS editor has been supplied to two clients for beta testing. Their initial reaction is quite positive and we expect to make this add-on product available in the near future.

An extensive review of the literature indicates that attribute modeling for kraft pulps is feasible and that the structure developed for mechanical pulps is applicable for kraft pulps. A report describing this work has been drafted and is being reviewed internally prior to publication as a project report.

STATUS

The release of version 3.0 allowed us to devote our efforts to the development of a more flexible, friendly data entry and editing process for μ MAPPs and to the extension of performance attribute modeling to kraft and other pulping processes. Maintenance and marketing continued to consume a significant fraction of our efforts.

Marketing Activities

The Helsinki University of Technology has chosen MAPPs to be the simulation package they will use in the current Linkage program. The Linkage program is designed to bring scholars and industry people to Helsinki University of Technology for a one-year course of study. The current program is titled Process Control and Management in the Pulp and Paper Industry and is planned for a group of 20-25 students. They will be using MAPPs for systems analysis of pulp and paper operations.

The "third world" represents a market largely untapped by current process simulation packages. We have had a number of information requests from many countries, but no success in selling MAPPs. We are in the process of establishing a marketing relationship with a consultant who serves the South American pulp and paper market (principally in Brazil and Chile). We hope this will enable us to sell MAPPs to a number of companies. In addition, we have recently sold a copy to the University of Guadalajara for use in their pulp and paper technology program. Hopefully this will lead to a demand for MAPPs in the future as these students enter the industry.

I am also pleased to report that Western Michigan University and Miami University have joined the MAPPS user community. We now have MAPPS in all the major pulp and paper schools with the exception of North Carolina State.

Maintenance Activities

As with any large program, maintenance work continues unabated. We have converted to using a program maintenance tool for our mainframe work and are investigating the use of such a tool for μ MAPPS. We are also investigating the use of CASE and expert system tools for code development, but have not found any satisfactory tools or systems to date.

Development Activities

Many of our users have commented that the current MAPPS editor is not "friendly" enough for novice users and that acceptance could be greatly improved through a menu-drive entry/editing facility. We have developed such a facility and it is in beta test. Concurrent with the beta test, we are developing the documentation for it. Our current plan is to market this tool as a μ MAPPS productivity tool and price it separately from the main program. We hope to have this program available in next two to three months. Mike Schreiter will demonstrate it at the meeting in October.

This program does not answer all of our users needs. In particular, it does not address the issue of allowing the user to enter data in "familiar", as opposed to MAPPS, units. We are considering how this might be done as an extension to either the current or new editor.

The coupling of an optimization package to MAPPS is still one of our development goals. We have made little progress in this area, but are continuing to explore how it might be done. We had hoped to write our own algorithm to ease the maintenance and licensing problems. We do not have the manpower to do that, so we are exploring the purchase and modification of existing software.

The ability to estimate product performance potentials for mechanical pulps was a significant addition to the version 3.0 of MAPPS. The extension of this capability to the kraft process is a nontrivial, but highly desirable or even necessary goal. The remainder of this report summarizes our efforts in this area.

MAPPS Performance Attribute Simulation

INTRODUCTION

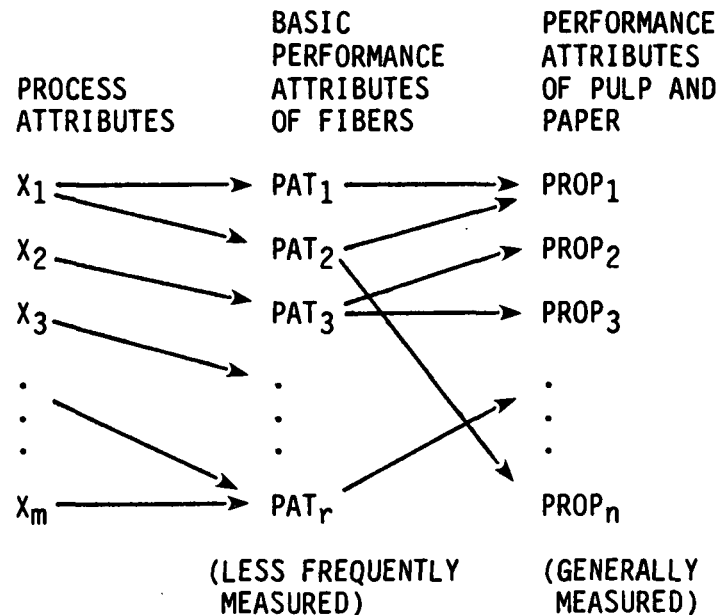
The literature of the pulp and paper industry is dominated by a discussion of the various testing methods and how they relate to end-use performance. A great deal of progress has been made in understanding and quantifying the fundamental relationships between important papermaking variables. These theoretical relationships have not yet been integrated into a comprehensive system of model equations useful for simulation.

Measures of performance vary widely. Many tests do not adequately represent actual behavior in use. Measurements of both elastic and failure mechanical, optical, and surface properties are widely applied measures of performance. Also anisotropy and sheet formation are important indicators of end-use performance.

As shown in Figure 1, performance attributes (PAT) are key variables of the fibers and network which link raw materials and processing conditions (X's) to measures of end-use performance (PROP's). PAT models provide the linkages between the X's and PAT's. Property models provide the linkages between the PAT's and the PROP's.

Figure 1.

PERFORMANCE ATTRIBUTE STRUCTURE



The PAT's must account for all or most of the major influences on performance: species, growth pattern, pulping, screening, cleaning, bleaching, additives, sheet forming, wet stretching, wet pressing, and drying. They should also account for environmental conditions during testing such as temperature and humidity. Ideally, the PAT's should also account for the anisotropy of the web such as MD/CD variation and sidedness.

The properties of handsheets and machine-made papers represent two benchmarks in comparing performance. There are three main differences between handmade paper and machine-made papers: (1) beating in a laboratory scale beater vs. a large scale disc or conical refiner, (2) handmade sheets with random orientation differ from oriented sheets developed through draws

which affect MD/CD directionality in properties and (3) uniformity in basis weight or formation which affects variation in properties.

Despite these apparent differences, the entire process is a continuum from high yield mechanical pulps to lower yield chemical pulps and from uniformly beaten and formed handsheets to rapidly refined and machine-formed papers as shown in Figure 2. Similarly sheet properties can be treated as a continuum with three major axes being densification, network anisotropy and intrinsic fiber properties as shown in Figure 3. The objective is to develop a unified model of papermaking along these lines. The following discussion interleaves the various factors which influence performance attributes from this point of view.

Figure 2

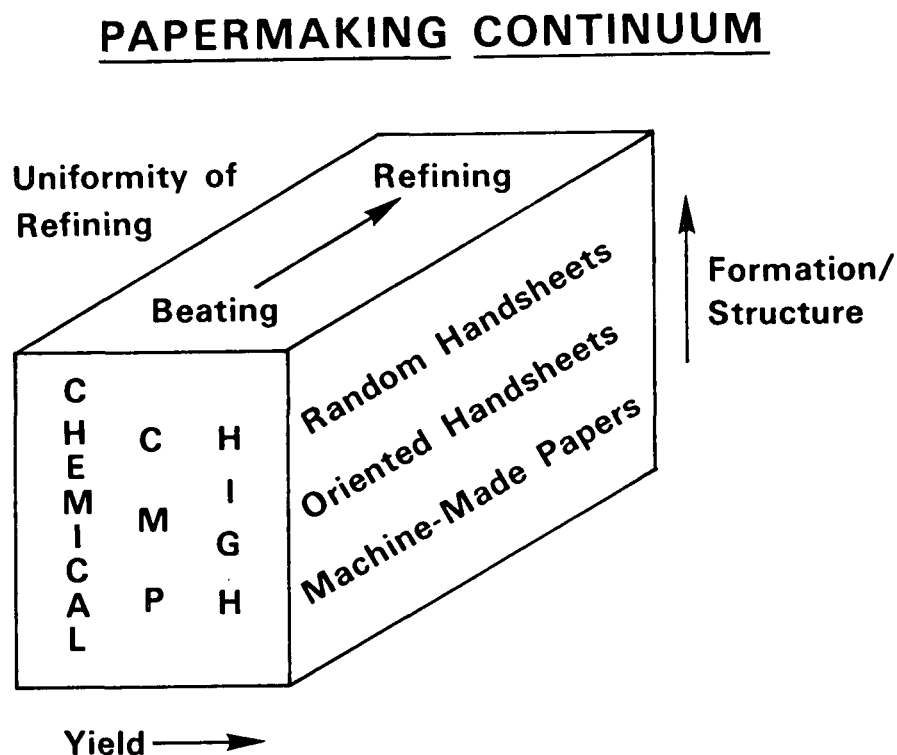
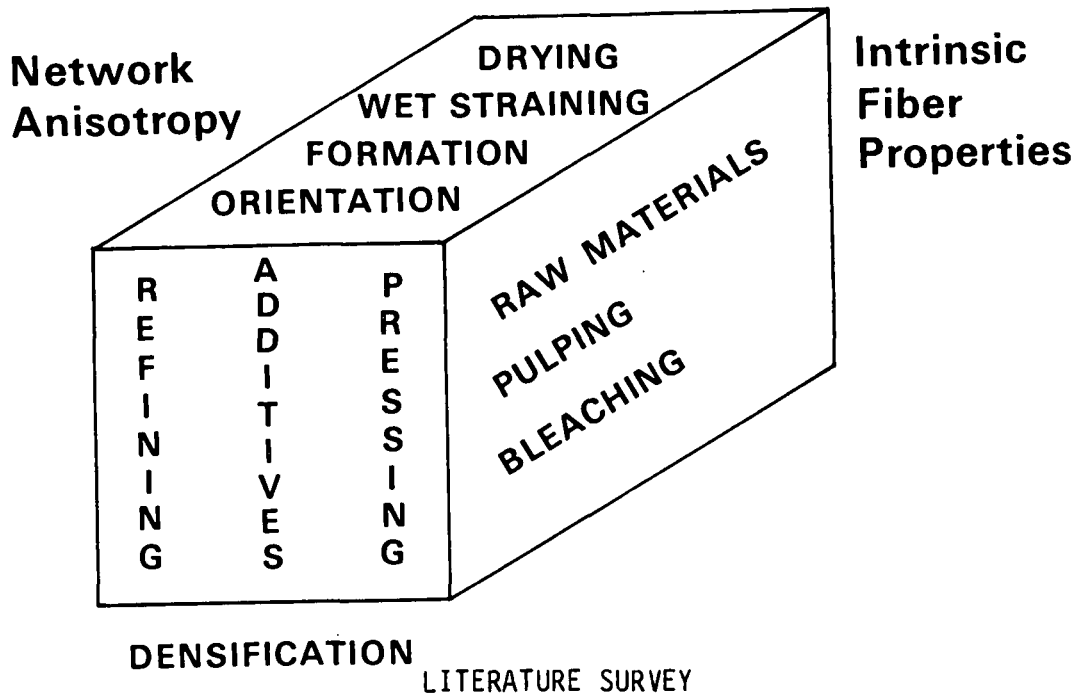


Figure 3

PROPERTY CONTINUUM

A nearly universal observation is the strong correlation between apparent sheet density and sheet mechanical (including both elastic and failure) and optical properties (Clark, Malmberg). Many important properties can be correlated quite well with just two variables, specific modulus of elasticity and apparent density (Malmberg) in terms of power law models. The few parameters in these models are relatively invariant with processing conditions.

Both specific modulus of elasticity, E and scattering coefficient are directly proportional to the increase in density of the sheet, $(d - d_u)$.

$$E = \text{const } (d - d_u) = \text{const } (SL - SL_u)$$

where d_u and SL_u represent the density and scattering coefficient of the

unbonded sheet. Other tensile properties which can be related to combinations of E and d through f defined as

$$f = E/d = (d-d_u)/d$$

include modulus of elasticity by bending, breaking length, elongation, tensile rupture energy, burst, and tear.

Structural theories (Cox, Page and Seth, Perkins and Mark) treat paper as a network of structural elements (fibers) connected at discrete points (bonds). These theories incorporate most, if not all, of the fundamental aspects affecting the mechanical properties of the sheet including the geometry of the network, fibers and bonds. Molecular theories (hydrogen-bond theory of Nissan) treat paper as a continuum of intermolecular covalent and hydrogen bonds. Although the structural theories explain much of the observed behavior of paper, they do not predict directly the influence of temperature and moisture content on paper properties which are a fundamental outcome of the molecular theories.

Nissan recently applied hydrogen-bond and percolation theory to show that specific elastic modulus is a function of sheet density which is consistent with the structural theories as modified below.

Page's structural model for the elastic modulus of the isotropic sheet is derivable from more fundamental small strain theories of orthotropic solids. Elastic modulus is proportional to fiber modulus, E_f , with corrections for bonding and shear modulus, G_f .

$$E = (1/3) * E_f * [1 - W * (E_f / (2 * G_f))^{1/2} / (L * RBA)]$$

where W is the average fiber width and L is the weight-average length.

The relative bonded area is defined in terms of the normalized light scattering coefficient, SL , relative to that of the unbonded sheet, SL_u .

$$RBA = (SL_u - SL) / SL_u$$

Including the effects of dislocations, microcompression, curl, crimps, and kinks, Page et al. arrived at the following general expression for E ,

$$E = (1/3) * E_f * [1 - W * ((n_f + 1) * (E_f / (2 * G_f))^{1/2}) / (L * RBA)]$$

where n_f , the number of separate regions in the fiber that are crimped.

Clark (1973), in analyzing the Page equation to reduce it to measurable quantities, maintains that RBA is proportional to apparent sheet density, d .

$$RBA = k^2 d * W / (t_f + W)$$

where k is the proportionality constant relating the fiber geometry and the number of fiber bonds per fiber. t_f and W are the fiber thickness and width respectively.

RBA is found to increase with beating time, breaking length and elastic modulus in agreement with the Page-Seth model. However, RBA may go through a maximum and then decrease with beating time while breaking length and modulus continue to increase.

Helle asserts that bonding strength which is mainly shear strength in accordance with the Page expression, tends to be higher in summer than in spring wood, that beating lowers bonding strength and that bonding strength decreases with yield. He finds that sulfite and sulfate pulps have nearly the same bonding strength. Bonding strength is roughly .5 to 1% of the tensile strength of the fibers. This indicates that

$$G_f = k * Z_f = k * Z$$

where Z is the zero-span tensile strength of the sheet which is assumed to represent average effective fiber strength in the sheet, Z_f .

Correlative models of sheet density indicate apparent density is a function of fiber density, fiber geometry and Canadian standard freeness or equivalently specific surface area. No fundamental models have been developed for sheet density.

Species and growth pattern (spring or summer) determine the morphological and chemical characteristics of the untreated fibers. Fiber strength, density, length, diameter, and composition (cellulose, hemicellulose and lignin content) are the primary factors. Other factors such as fibril angle are a measure of intrinsic fiber strength. Also important are fiber flexibility which is proportional to fiber coarseness, cell wall thickness and lumen diameter.

Degree of digestion and the digestion process itself influence zero span tensile strength, bending stiffness, coarseness, and length of fibers. The effect on fiber length is not felt until the fibers are refined. The effects of reduced yield on the refined pulp are felt indirectly through changes in fiber density and stiffness. The result is that sheet breaking length at first increases and then decreases with decreasing yield. The maximum depends on the trade-off between surface area development which increases sheet density and decreasing fiber density and strength, which decreases strength and modulus.

The radial distributions of hemicellulose and lignin influence the degree of surface area development, swelling behavior and wet compressibil-

ity. For example, lignins are distributed evenly in the sulfate pulps while in sulfite pulps they predominate in the outer layers. The result is that sulfite pulps beat more easily and independently of the degree of digestion. The sulfate pulps beat more slowly and show a more marked dependence on the degree of digestion.

Removal of lignin and cellulose components affect fiber density directly. Fiber strength and elastic modulus are reduced by the extent that cellulose and hemicellulose are degraded.

Fiber length and width distributions can be approximated as normal or log-normal. Weight average fiber length and diameter are not markedly changed in the pulping step. What reduction that does occur comes about because defects introduced during pulping and bleaching manifest themselves during refining.

The primary influences of refining are to increase fiber surface, specific volume and flexibility. Indirectly, fiber length distribution is also affected. Fiber strength, compliance or flexibility and spring back affect sheet bulk, density or relative bonded area.

Bond strength as measured by shear stress or shear strength also increases with beating and refining. This may be a direct effect of surface area development or it may represent an indirect measure of the increased conformability of the fibers which is also improved by refining. These factors in turn influence sheet mechanical properties.

The principle independent refining variables are net specific power, NSP, tackle design, fiber conformability and composition, and consistency.

Net specific edge load, NSEL, conveniently combines the effects of tackle with NSP. Miller shows that for high yield pulps NSEL is more applicable than NSP. Kraft pulps are relatively insensitive to NSEL but are sensitive to NSP.

Differences between beating and refining are reflected in the distribution of specific surface over fiber length. Differences between chemical pulps and high yield pulps are reflected in the fiber flexibility for a given power input. The other difference is that specific surface in high yield pulps is more a function of fibrillation and fines formation which shows up in reduced freeness. Specific surface in chemical pulps results in more uniform fibrillation and far less fines formation.

The kinetic models based on the work of Yan currently used for mechanical pulping which relate length and width distributions to NSP should be applicable to chemical pulps. In addition the K-factor model for specific surface area development enables the effects of nonuniform treatment to be included. This allows for a continuum of conditions to be modeled from uniform beating to highly nonuniform refining. In addition, the effects of NSP, consistency and the specific surface of the entering stock are taken into account in these models. Miller developed a correlation for net specific power consumed in terms of throughput, rpm, consistency and gap.

Stationwala and Atack show that natural log Canadian Standard Freeness (CSF) is directly proportional to the hydrodynamic specific surface for high yield pulps. The relationship is found to be linear for chemical pulps (Yan). As the mat is compressed under an applied load, P , the density increase, d , is of the form:

$$d = M \cdot P^N$$

M and N are compressibility constants which are characteristics of a given pulp. Cowan showed that N increases with decreasing CSF and M increases with decreasing yield. This implies that decreasing CSF is also related to increasing fiber conformability.

During drying there are at least two forces leading to shrinkage: increased surface tension between fibers as inter-fiber water is removed (Campbell effect) and fiber shrinkage as intra-fiber water is removed. Bonding between fibers occurs as inter-fiber contraction proceeds and transmits the effect of intra-fiber contraction throughout the network.

Intra-fiber contractions manifest themselves mainly in a reduction in fiber diameter or width and thickness. There is very little change in fiber length as a result of removal of intra-fiber moisture.

Tension applied during drying affects the shrinkage and expansion of paper but only over the moisture range which occurred during the application of the tension. Tensile strength and elastic modulus are increased by drying under tension due to the formation of a tighter bonding pattern and more uniform stress loading in the direction of the applied tension.

Bulk does not change significantly with restraint for unrefined or high freeness kraft and only slightly with increased refining. Both porosity and elastic modulus vary substantially with restraint and the effect appears to increase with decreasing freeness. Starch addition has very little effect on bulk or porosity but does affect elastic modulus.

Orientation and the effects of stretch are similar and complementary. Orientation serves to distribute stresses in the direction of orientation while stretch serves to make the stresses more uniformly distributed over the

sheet in the direction of application. Orientation leads to an increase in strength in one direction and a corresponding reduction in the normal direction. Stretch has a similar effect since the stresses are applied more uniformly in the applied direction with increased stretch. Stress redistribution appears to occur at both the inter and intra-fiber level.

Both tensile index and modulus increase, pass through a maximum and then decrease with increased stretch during wet straining and drying. Both the overall levels and the relative height of the maxima increase with increasing orientation angle. All the maxima occur at approximately 1% stretch (Setterholm, Kuenzi, Parsons). The height of the maxima increases with increasing orientation angle indicating an interaction between stretch and orientation.

Beyond 1% stretch both strength and modulus decrease at all orientations. One proposed cause is the reduction in RBA due to the pulling away of adjacent fibers. It appears reasonable to assume that the main influences of orientation and stretch during wet straining and drying are felt in the MD/CD ratio of breaking length and modulus.

One measure of formation is inhomogeneity in density which may result from basis weight and thickness variations. Macro-scale density variations result from variations in fiber floc size which are caused by a variety of factors such as the balance between electrostatic and hydrodynamic forces during dewatering.

Variations in density lead to corresponding variations in tensile and optical properties of the sheet. Increased formation variation (i.e. density variation) increases the coefficient of variation, CV, of all tensile and optical properties about their mean values and affects average property values.

In general the CV values reach optimal (minimum) levels for many mechanical properties at specific conditions (Graber and Gottsching 1979). CV values tend to be lowest at or near the normal machine operating conditions. For example, CV values were minimal for jet/wire ratio of 1.08. CD CV values were generally less than MD CV values. Machine speed had surprisingly small influence on MD CV in basis weight and thickness. However, also surprising, CD CV for many properties decreased with increasing speed.

CV values tend to be lower for the high turbulence headbox than the standard design. The trends for this headbox are similar to those of the standard design, i.e. the MD and CD basis weight CV tends to decrease with increasing machine speed, and the optimum in jet wire ratio remains near 1.08.

Wire shake tends to increase fiber orientation in the machine direction. Increased amplitude and frequency of oscillation increase the length over the width of the orientation ellipse (Danielsen). Shake is intended to make the formation more uniform. Thus the CV of density is expected to decrease with various combinations of shake frequency and amplitude.

Dewatering and drainage are of course extremely important processes on

the wire. This area has been extensively studied but there is still no simple model of this process which could be amenable to performance modeling. The current approach to modeling this area (i.e. clarifiers and splitters) will represent the process adequately for our current needs.

Porosity is related to the size of the pores and is clearly related to the sheet density and basis weight. Pore size decreases with increasing basis weight (Van den Akker, 1978) and with increasing sheet density at any given basis weight.

The Kubelka-Munk theory of light transmission is generally regarded as a reliable model of the optical properties of most papers (Bristow and Kolseth, 1986). Reflectivity as given by the K-M theory is related to the ratio of absorption coefficient, k , to specific scattering coefficient, SL , by the following,

$$r_{inf} = 1 + (k/SL - ((k/SL)^2 + 2*(k/SL))^{1/2})$$

or conversely,

$$k/SL = (1 - r_{inf})^2 / (2 * r_{inf})$$

The printing opacity is the ratio r_0 to r_{inf} . The color is the value of r_{inf} at a given wavelength and the brightness is the value of r_{inf} at 457 nm.

The scattering coefficient may be estimated from the sheet density using the Malmberg correlations since these appear to be accurate at the specific scattering typical of bleached pulps.

The linkage between scattering coefficient, RBA and sheet density indicates that bleaching has an effect on optical as well as mechanical proper-

ties of the sheet. The data confirm that the handsheet sheet density must increase as a result of bleaching. Bleaching should soften the fibers allowing the fibers to collapse more readily into a ribbon-like structure. However the influence of bleaching is controversial.

Giertz concluded that bleaching reactions do not influence the opacity properties of the pulp. Scattering coefficient of the bleached pulp is the same regardless of the bleaching method. This indicates that density is not greatly affected by bleaching.

However, when opacity is expressed as contrast ratio or print opacity, opacity is lowered by bleaching. Conditions which lead to an increase in density of the sheet will also generally increase the opacity.

PROPOSED PERFORMANCE ATTRIBUTE MODELS

The data show that once density is known, most other properties can be predicted with a reasonable level of certainty. Sheet density is determined by packing "efficiency". This is affected by fiber conformability and by the ability to fill in the interstices within the voids. In mechanical pulps, these interstices between the stiff and rod-like fibers are filled with fines and fibrillar material. Sheets made from chemical pulps have fewer voids because the fibers are compressed and flattened into ribbons which form layers with fewer voids. Fewer fines are generated during refining because of the lower power used and higher fiber conformability in the shear field of the refiner. Bonding strength or bond frequency tend to be higher in the chemical pulp than in the mechanical pulp due to contact of flattened lignin-

free fiber surfaces. Not only are the fibers packed in intimate contact, they are also bonded together. This means that the packing density is a condition which should be present for a strong sheet but is not the only condition. Even if the interstices are filled with fine particles as in the case of mechanical pulps, in the absence of strong bonds, the sheet strength will be low.

It is possible to increase sheet density without increasing tensile strength or elastic modulus. The Malmberg relationships confirm that as density reaches a limiting value (say that of cellulose), tensile strength does not continue to increase. For example, addition of fines generally increases sheet density although it may not always increase bonded area and strength.

Density Model

For a two phase system in which water is the continuous phase, we more properly have a slurry and the density of the slurry can be obtained in a straightforward fashion from the consistency and the total mass flow rate.

At some consistency, fibers become the continuous phase and we can speak of a sheet rather than a slurry. What follows applies to the sheet above a certain critical solids level. This would occur presumably at the dry end of the paper machine.

Bulk density depends on the packing efficiency and the intrinsic density of the individual components. On the scale of the fiber network, we can think of the network as made up of two components, fibers and voids. On the scale of the individual fibers, we can think of the fiber density as consisting of two components, solids containing cellulose and hemicelluloses and

water-filled voids. The densely packed, relatively dry sheet has two main components

$$d = (1-e)*d_f + e*d_v$$

where d_v is the density of material in the voids and e is the void fraction.

For a suspension of water-swollen fibers, d_f and d_v are nearly equal to that of water and $d = 1.0$. As the moisture is removed, the sheet becomes compact and the fibers shrink, d_f increases and d_v decreases, until we reach a condition for which

$$d = (1-e)*d_f$$

Fiber Density

The bulk density of the fibers varies considerably during processing. At any given time, the fibers are composed of solids and voids.

$$d_f = (1-e_f)*d_s + e_f*d_v$$

where

d_s = density of the solids (cellulose, hemicellulose,
and lignin)
 d_v = density of the material in the voids
 e_f = intra-fiber void fraction

The intra-fiber void fraction is negligible for untreated fibers. The solid density is a function of the densities of cellulose, lignin and hemicellulose.

$$1/d_s = X_c/d_c + X_l/d_l + (1-X_c-X_l)/d_{hc}$$

where

X_c = mass fraction cellulose
 X_l = mass fraction lignin
 d_c = density of cellulose
 d_l = density of lignin
 d_{hc} = density of hemicellulose

We assume that there are only three components, cellulose, lignin and hemicellulose within the solid fraction. Moisture would occupy the void fraction.

As a result of pulping and bleaching, d_f is changed by the removal of most of the lignin and some of the cellulose and hemicellulose.

Removal of lignin from the outer layers of the fibers allows the fibers to swell through absorption and adsorption of water. Application of pressure and removal of intra-fiber water during drying tends to cause the fibers to collapse into ribbon-like structures. Thick-walled fibers will have less tendency to collapse than thin-walled fibers. Thus the void fraction within fibers and the fiber bulk density will vary with species, pulping and bleaching conditions, and moisture content.

For air-filled pores, d_v may be neglected and

$$d_f = d_s(1 - e_f)$$

e_f depends on the collapsibility of the fibers and approaches zero for a highly beaten, low yield fiber as water is removed. In the limit, the fiber density approaches that of cellulose,

$$d_f = d_c$$

Sheet Density in Terms of Relative Bonded Area

According to Clark's analysis of the Page relation,

$$RBA = k * W * d / (t_f + W)$$

Since RBA is dimensionless and d has the units of density, k must have the units of $1/d$.

$$k \propto 1/d_f$$

Then solving for d,

$$d \propto d_f \cdot RBA \cdot (t_f + W) / W$$

It is also reasonable to assume that as RBA approaches 1.0, d approaches d_f and

$$d \propto d_f \cdot RBA .$$

Comparing the expression above for d with that involving e and neglecting the contribution due to the voids, we see that

$$1 - e \propto RBA$$

Density in Terms of Hydrodynamic Specific Surface

Observe that d increases with the degree of beating and refining. Clark and others state that RBA is proportional to the hydrodynamic specific surface, S_h , developed during refining. Since we also know that density, strength and elastic modulus increase during wet pressing, we assume further than RBA increases during wet pressing. Thus RBA is some function of the specific bonding area, S_b , which is related to S_h .

$$RBA = f(S_b)$$

After refining and prior to wet pressing and drying,

$$S_b = c \cdot S_h .$$

c is less than one and may depend on fiber geometry and conformability (coarseness).

For unrefined pulps, S_b is low, (about 1) and RBA is proportional to S_b . As S_b increases, RBA becomes less dependent on S_b and approaches 1 asymptotically. This suggests a function of the following form.

$$RBA = S_b / (k_1 + S_b)$$

Combining the relationships above and eliminating RBA, we obtain the following model for d in terms of the fiber density and the specific bonding surface area.

$$d = d_f * S_b / (k_1 + S_b)$$

For unbonded sheets, d approaches d_u which varies from .3 to .4 for chemical pulps and is lower for high yield pulps. It is assumed that d approaches d_u as S_b approaches S_u which is approximately 1.

Solving for k_1 , we obtain,

$$k_1 = S_u * (d_f / d_u - 1)$$

The resulting model for d is as follows,

$$d = d_f * S_b / (S_u (d_f / d_u - 1) + S_b)$$

Surface Area Model

Employing the K-factor model used for mechanical pulping, S_h is expressed in terms of fiber length distribution and K factor,

$$S_h = 1 - \sum_{i=1}^n (X_i * \ln(L_i / L_a)) / K$$

and the K-factor accounts for variations due to uniformity and extent of refining, species and pulping.

$$K = K_0 * e^{(k_2 * NSP)}$$

k_2 is a function of consistency, species, kappa number and inlet K-factor, K_0 . L_a is a typical average fiber length.

Σ represents the summation over all fiber length fractions i from 1 to n . K decreases as NSP (net specific power) increases. As K decreases, S_h tends to increase for fibers shorter than L_a and decrease for fibers longer than L_a .

For sufficiently high values of NSP, K may increase thus simulating fiber cutting which does not contribute to surface area development. S_h may also change due to the reduction in fiber length distribution during refining.

Refiner Model

The refiner model uses statistical distribution functions to model the changes in fiber length and width during refining. The fiber particle categories are related to combinations of length and width. The mean and standard deviation of the particle length and width are changed by the net specific power (NSP) applied to the refiner based on models from Yan (1975).

$$L = A_1 + (L_{in} - A_1/A_2)\exp(-AL_1*ZP)$$

and

$$\sigma_L = A_1 - A_2/L$$

where

$$ZP = 10(NSP - A_p)/B_p$$

Similar expressions apply to the width parameters, W and σ_W .

Freeness Model

The Canadian Standard Freeness model is based on the equivalence between S_h and CSF according to the work of Stationwala et al. (1979).

$$S_h = S_1 - S_2*\ln(CSF)$$

Thus

$$CSF = e^{(S_1-S_h)/S_2}$$

Fiber Fractionation

The fractionation model has three roles: pressure screen, centricleaner

and thickener. Separation of fibers in the pressure screen and centricleaner is based on the length and width of each fiber type. The algorithms currently used in the mechanical pulping module HYFRAC, are assumed to apply to chemical pulps as well. The two adjustable parameters in each model will account for design, operating conditions and fiber conformability.

In general the screen separates mainly on fiber length while the centricleaner separates on width or length to width ratio. There is also an indirect separation on the basis of specific surface area. The cleaner also separates on density of debris and dirt. Performance attributes are "separated" into accepts and reject attributes based on conservation of specific surface or other principles which may apply to an attribute.

Fiber Mixing

Stock mixing will be handled in the same fashion as mechanical pulps. Performance attributes such as length and width distribution statistics, CSF, K-factor and absorption coefficient are mixed based on appropriate mixing rules. For example, mixing of CSF is based on conservation of hydrodynamic specific surface. Length and width mixing is based on conservation of mass and volume. Most other mixture attributes are based on weight averaging.

Density Effects During Wet Stretching

Density increases during drying mainly by the Campbell effect (surface tension). This effect is accounted for indirectly through the surface area model assuming that surface tension itself is lumped into of S_h and is relatively constant from system to system.

Densification Through Pressing

During wet pressing density increases due to the mat compressibility.

$$d = d_i + M \Delta p N$$

However, it could be assumed that what actually increases during wet pressing is the bonded area, S_b and density is increased indirectly.

$$S_b = S_{b0} (1 + M \Delta p N)$$

where S_{b0} into the first press nip is equal to S_h determined from the combined effects of refining and stock preparation.

$$S_{b0} = C S_h$$

N is approximately linear with freeness, CSF, which we represent by specific surface, S_h .

$$N = N_1 + N_2 S_h$$

M is a function of yield

$$M = M_1 + M_2 Y$$

where M_2 is negative.

Model for Elastic Modulus in Terms of Density

Page defines RBA in terms of SL , specific light scattering coefficient,

$$RBA = (SL_u - SL) / SL_u$$

Malmberg found a linear relationship between light scattering coefficient and d .

$$SL_u - SL = k_4 (d - d_u)$$

where k_4 is approximately equal to SL_u .

Eliminating SL from the expression for RBA, we obtain an expression which shows that relative bonded area is directly proportional to the

increase in sheet density over that for the unbonded sheet.

$$RBA = (d - d_u)/(1 - d_u)$$

Thus as d approaches 1 (greaseproof paper), RBA approaches 1.

Combining the Page model for elastic modulus of the isotropic sheet, E_{iso} , and the relationship between RBA and scattering coefficient and the Malmberg correlation between scattering coefficient and density, we obtain a relation between E_{iso} and d ,

$$E_{iso} = (1/3)E_f * (1 - (1 - d_u) * W * (E_f / (2 * G_f))^{1/2} / (L * (d - d_u)))$$

which is valid for

$$d > d_u + (1 - d_u) * W * (E_f / (2 * G_f))^{1/2} L.$$

Otherwise $E_{iso} = 0$.

Fiber Geometry

Initially, the species data base will determine W and L typical of a given species. For mechanical pulping, the chips will flow into the primary refiner and emerge with average length and widths consistent with the above values. W will more properly be the original diameter of an approximately cylindrical fiber. As fibers collapse the width will change. The final fiber dimensions will influence the properties through the terms in the equation for elastic modulus.

The thickness of the collapsed fiber, t_f , is related to the cell wall thickness of the fibers, CWT ,

$$t_f = 2 * CWT$$

where CWT is also defined by species and growth pattern.

The perimeter, p , for a flattened, ribbon-like fiber is then defined as

$$p = 2*(t_f + W)$$

and cross-sectional area, A, is defined as

$$A = W*t_f$$

L refers to the weight-average length and W to the number-average width of the fibers. The parameters for the refining of chemical pulps will be determined so that L is approximately equal to the reference length, L_r , which is the average for the species and growth pattern defined in the data base.

The width is determined as follows. For the unrefined fiber, the fiber width and diameter are the same and the fiber is assumed to have a circular cross-section (i.e. no thickness). The reference perimeter, p_r is defined as,

$$p_r = \pi * D$$

where D is the reference fiber diameter which is a function of species and growth season and is obtained from the data base.

Flattening of the fiber is assumed to preserve the fiber perimeter.

$$p = p_r$$

This allows the reference width of a flattened fiber, W_r , to be computed in terms of the perimeter,

$$W_r = p_r/2 - 2*CWT$$

Parameters in the refining of chemical pulps are determined so as to produce an average fiber width approximately equal to the reference width, W_r .

Bond Strength

Shear modulus is assumed to be a measure of the bond strength between fibers. Since intra- and inter-bond strength is a strong function of hydrogen bonding between cellulose molecules, it is reasonable to assume that the bond strength is linearly proportional to the intrinsic fiber strength which is assumed to be proportional to the zero-span tensile of the sheet.

$$G_f = c \cdot Z_f = c' \cdot Z$$

Determination of E_f in Sheet Modulus Model

As shown by Krause, fiber strength, as measured by zero-span tensile, decreases with decreasing yield for sulfate pulping. Actually, zero-span tensile decreases in a linear fashion with the reduction in cellulose and hemicellulose. This is the difference between the yield reduction and the kappa number reduction with the appropriate change in units.

As a first approximation, Z is given as Z_f , the strength of the untreated fiber, multiplied by a linear term to represent the reduction due to loss of cellulose and hemicellulose, DC.

$$Z = Z_f \cdot (1 - k \cdot DC)$$

where k can be approximated by the average slope of the strength reduction data of Alexander and Marton.

The term E_f in the equation for elastic modulus is analogous to Z and Z_f in the Page equation for tensile strength. It is reasonable to assume that models which apply to Z also apply to E_f . Thus E_f is reduced by removal of cellulose and hemicellulose during pulping and bleaching (Helle).

$$E_f = E_{fu} \cdot (1 - k' \cdot DC)$$

where E_{fu} is the tensile modulus of the untreated fiber.

Sheet Anisotropy

The elastic modulus computed by above model is the isotropic modulus, E_{iso} . In machine-made paper E varies in the MD and CD and it is assumed that E_{iso} is the geometric mean of the moduli in each direction.

$$E_{iso} = (E_{MD} * E_{CD})^{1/2}$$

Effect of Orientation

Another factor which affects both Z and E_f is orientation and stretching during drying. For a given amount of stretch, E_{MD} is a linear function of OR when plotted on log-log coordinates.

$$\ln(E_{MD}) = a * \ln(OR) + b$$

OR is the orientation ratio defined as

$$OR = \cotan(\theta)$$

θ must either be specified or determined from a correlative model. Reasonable values can be easily specified. A typical paper machine will operate with a relatively constant value of OR. It would be desirable to link OR to machine operation such as rush/drag ratio, wire speed and head box for consistency. a and b must incorporate the effects of stretch and pulp type.

Setterholm found that as OR increases, E_{MD} is more sensitive to stretch, s . Although E_{MD} increases more steeply with s as OR increases, it still levels off at roughly the same value of s . Beyond this it may tend to decline. This suggests the following preliminary model for E_f to include the influence of stretch and orientation, (Gates, Sapp and Gillespie, Setterholm, Chilson, Setterholm, Kuenzi, Parsons).

$$R = E_{MD}/E_{CD} = c \cdot OR \cdot (1 + k \cdot (s - s_0))$$

where c is approximately 1.09, k is approximately -.0054, s_0 is the stretch (+) or shrinkage (-) in %. and s_0 is about -12%.

Combining the relations for E_{iso} and E_{MD}/E_{CD} , we obtain

$$E_{MD} = E_{iso} \cdot R^{1/2}$$

The above model for E_{iso} takes into account the effects of species and growth patterns, pulping and bleaching, refining and, densification. R then accounts for the effects of orientation and stretching during wet straining and drying.

Property Models

The models for E (E_{iso} , E_{MD} or E_{CD}) and d are then combined through the power law models of the form

$$\text{Property} = a(E \cdot t)^b = a \left(\frac{E}{d} \right)^b$$

to obtain a variety of mechanical and optical sheet properties.

Property Models Including the Influence of Formation

The CV values for density measured by Gottsching could provide the basis for determining CV values for all other mechanical properties.

For example, the Malmberg correlations show that burst factor is a nonlinear function of sheet density and elastic modulus.

$$B = k \cdot (f/d)^3$$

where

$$f = E/d$$

Thus,

$$B = k*(E/d^2)^3$$

Now the variation in d is defined in terms of its mean, d_a and coefficient of variation, d_{cv} ,

$$\Delta d = d_a(1 \pm d_{cv})$$

where d_a is the base value determined by the models above. Thus d can assume a maximum or a minimum (not true maxima or minima) as follows,

$$d_{max} = d_a(1 + d_{cv})$$

and

$$d_{min} = d_a(1 - d_{cv})$$

Now substituting d_{max} and d_{min} into B above and defining B_{max} and B_{min} ,

$$B_{max} = k*(E_{max}/d_{max}^2)^3$$

and similarly for B_{min} . E_{min} and E_{max} are defined in terms of the elastic modulus model (iso, MD or CD) evaluated at d_{max} or d_{min} respectively.

Actually, there is no way, to determine whether the derived properties will be maxima or minima. The notation is based solely on d .

The reported properties could include the mean as well as the max and min. This would provide a range of expected property values about the mean of each value.

d_{cv} is affected by jet/wire drag ratio (minimum at 1.08), headbox turbulence level (impossible to quantify at this point), stock consistency, machine speed and wire shake. All the factors were evaluated over relatively small ranges by Gottsching but the results serve as a useful basis for very simple models to account for these factor. Again, adjustable constants are

used to account for design details.

The following simple correlative model is suggested

$$d_{cv} = A*MS + B*MS^2 + C*JWR + D*JWR^2 + E*CO + F*CO^2 \\ + G*(SA*SF) + H*(SA*SF)^2$$

where

MS = machine speed
JWR = jet-wire ratio
CO = head box consistency
SA = shake amplitude
SF = shake frequency

Specific scattering coefficient is also determined from the Malmberg correlation. The absorption coefficient is either given or assumed to be proportional to pulp lignin content. The change in absorption coefficient is assumed to be proportional to the reduction in lignin in each bleaching stage. Having the absorption and scattering coefficients, brightness is computed from the K-M theory described in the section on optical properties.

The Malmberg models include the following mechanical and optical properties: modulus of elasticity, bending modulus, breaking length (used to compute density), elongation, tensile rupture energy, burst factor, tear factor, and scattering coefficient. All of these can then be used to estimate these properties in terms of d and E.

Other mechanical properties not modeled directly by Malmberg such as various compressive properties (Ring Crush), converting properties (printability), optical and surface properties (opacity, porosity) can be estimated from simple correlative models where available (Kellogg, Thykeson).

The following 15 performance attributes are required for the chemical pulping and papermaking simulation areas:

- Kappa Number
- Fiber length and standard deviation
- Fiber Width and standard deviation
- Fiber density
- Zero-span tensile (fiber tensile, Z)
- Fiber elastic modulus (E_f)
- Canadian Standard Freeness (related to S_h)
- K-factor
- Bonding Area, S_b
- CV of apparent sheet density (formation)
- R (MD/CD ratio for elastic modulus)
- Absorption Coefficient
- Process Flag vector to incorporate the cumulative effects of species, pulping, and bleaching

Figures 4 and 5 illustrate the application of Figure 1 to describe some of the interactions possible in the PAT system. Figure 4 shows how raw materials (species or X's) influence intrinsic fiber properties which in turn influence end-use performance (PROP's) in this case tensile, scattering coefficient and brightness. Refining influences sheet density and affects various PAT's and PROP's in other ways. Wet pressing, drying, stretch and sheet forming would affect different PAT's (not shown). All of these effects would cascade and interact through the sequence of processing steps to influence all the end-use performance characteristics.

Figure 4

Relationships Between Process Variables, Performance Attributes and End-Use Performance

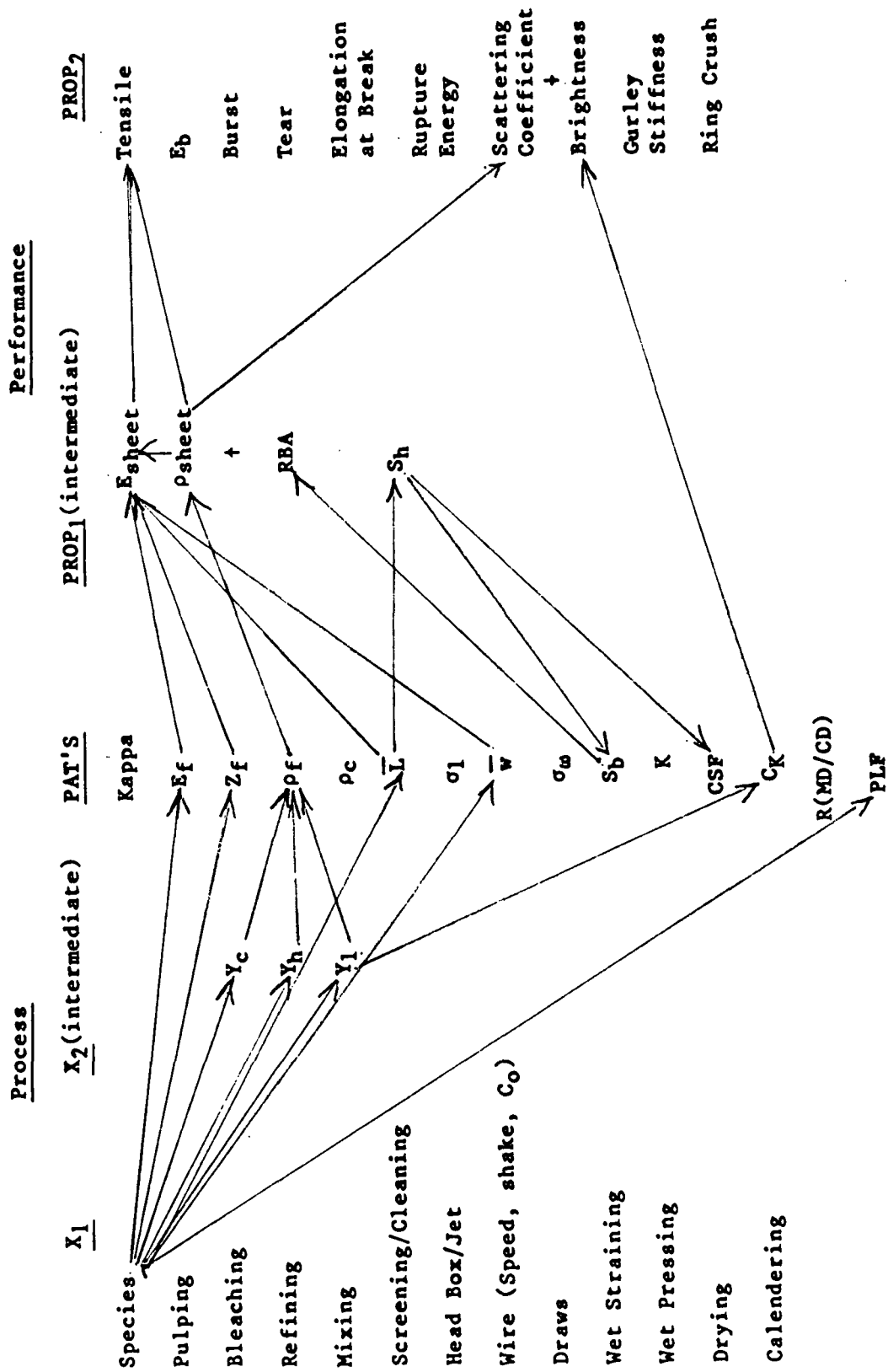
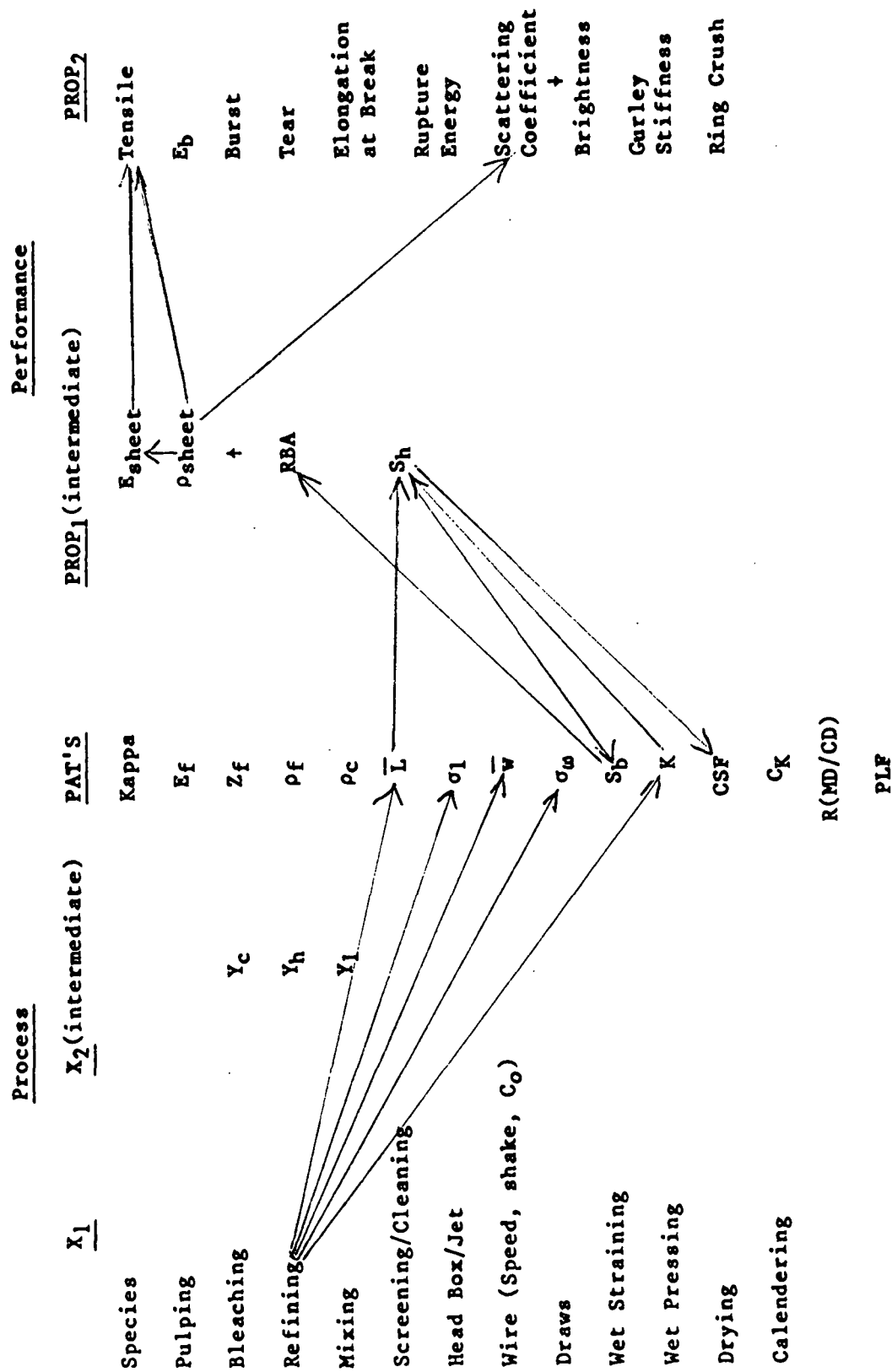


Figure 5

Relationships Between Process Variables, Performance Attributes and End-Use Performance



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NOMENCLATURE

A	fiber cross-sectional area
B	burst
CD	cross machine direction
CO	consistency
CSF	Canadian Standard Freeness
CV	coefficient of variation
CWT	cell wall thickness
d	density
D	fiber diameter
DC	fractional reduction in cellulose and hemicellulose
e	void fraction
E	modulus of elasticity
f	E/d
G	shear modulus
JWR	jet-wire ratio
k	light absorption coefficient
K	K-factor
Kappa	Kappa Number
L	fiber length
MD	machine direction
MS	machine speed
NSEL	Net specific edge load
NSP	Net specific power
OR	orientation ratio

p fiber perimeter

P pressure

PROPERTY sheet mechanical or optical property

r light reflectivity

R ratio of MD property to CD property

RBA relative bonded area

s stretch or elongation

S specific surface area

SF shake frequency

SL light scattering coefficient

t thickness

W fiber width

X mass fraction

Y yield

Z tensile strength (zero-span)

ZP normalized refiner residence time

Greek

ΔP change in pressure

θ orientation angle

subscripts

a average

b bonded (area)

c cellulose

CD cross-machine direction

cv coefficient of variation

f fiber

hc hemicellulose
h hydrodynamic (specific surface area)
i fiber index
inf refers to an opaque object
iso isotropic
l lignin
L length
min property evaluated at d_{\min}
MD machine direction
max property evaluated at d_{\max}
p power
s solid sheet
u unbonded
v voids
0 entering value

SYSTEMS ANALYSIS PROJECT ADVISORY COMMITTEE

and

MAPPS USERS GROUP

SLIDE MATERIAL

October 27-28, 1987

STATUS

VERSION 3.0

Marketing

Performance Modeling

The User Friendly Interface

The Optimizer

VERSION 3.0

Released in April

Contains Preliminary Performance Models

Delivered With Utilities for Local Customization

MARKETING

Four New Customers

Total Clients Is 29

MAPPS Will Be Used in TAPPI Video Course

Initial Penetration to Foreign Markets

PERFORMANCE MODELING

Interest Quite High in Current Capabilities

Extending To Cover More Processes

USER FRIENDLY INTERFACE

Development Driven By User Needs

IBM Compatible PC Only

Evaluated One Commercial Package

Elected Do Internal Development

USER FRIENDLY INTERFACE

Currently In Beta Test

Documentation In Preparation

Release In Late December

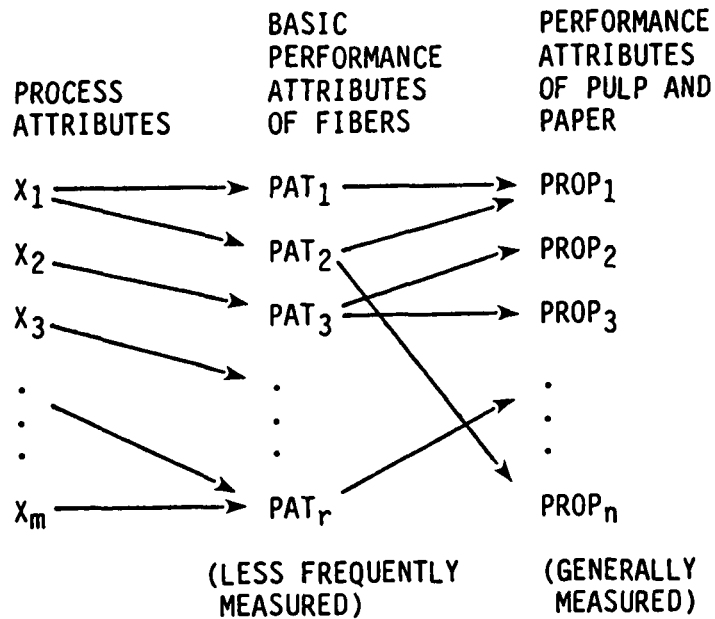
Additional Cost Item

OPTIMIZER

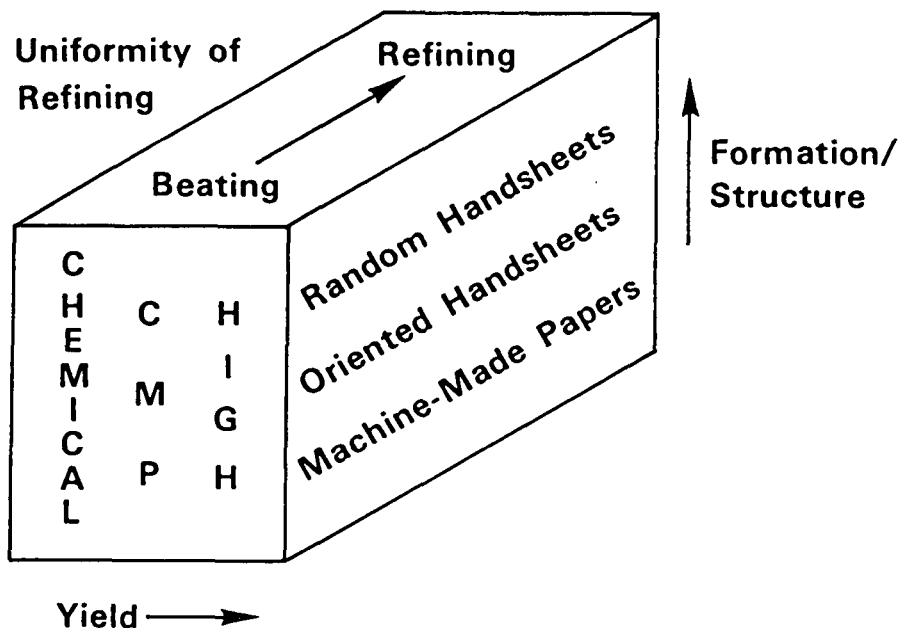
Insufficient Manpower To Do Own Development
Continuing to Evaluate Third-party Packages
Will Combine With Modified Version of Saffran's Interface
Low Level Of Effort -- Release In Summer (?)

MAPPS PERFORMANCE ATTRIBUTES SIMULATION

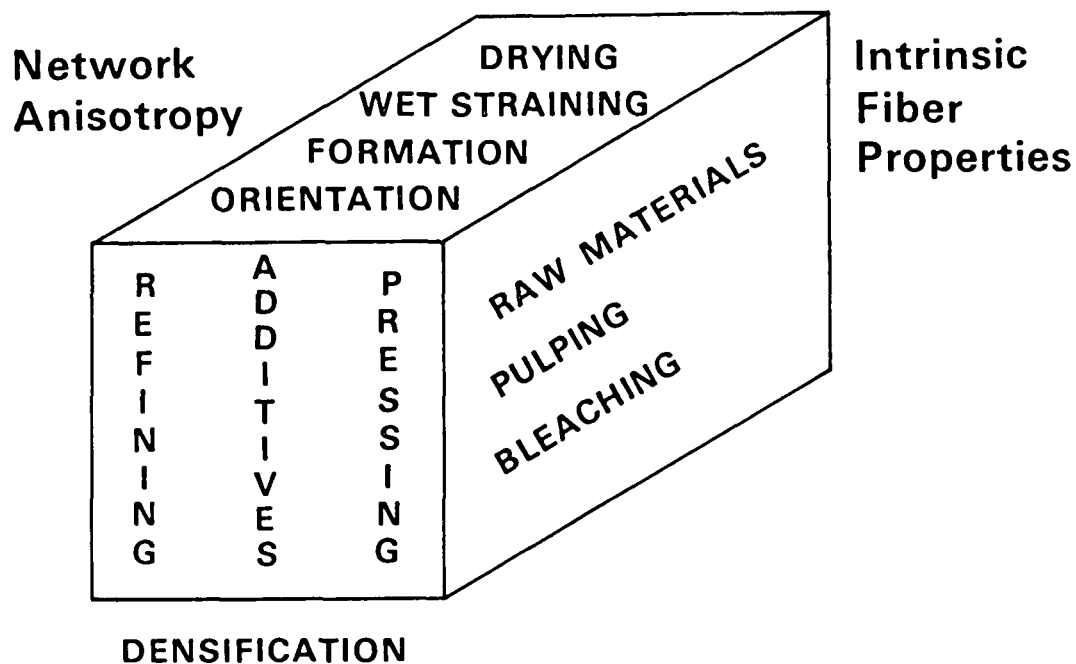
PERFORMANCE ATTRIBUTE STRUCTURE



PAPERMAKING CONTINUUM



PROPERTY CONTINUUM



GOAL:

Develop a unified model of performance development during pulping and papermaking.

LITERATURE

- * Property Models
- * Bonding
- * Fiber Properties
- * Effects on Elastic Modulus
 - pulping
 - refining
 - forming
 - wet pressing
 - drying

CORRELATIVE MODELS

- * $\text{Property} = f(\text{fiber density, fiber geometry})$
- * Parameters: yield, kappa, species, CSF
- * Specific to certain conditions

POWER-LAW MODELS (CLARK, MALMBERG)

variables: apparent density, elastic modulus

$$E = \text{const } (d - d_u)$$

$$\text{PROP} = f(E, t) = f(E/d) = f((d - d_u)/d)$$

POWER-LAW MODELS

$$\text{PROP} = a \cdot (E/d)^b$$

- * bending modulus
- * breaking length
- * elongation at break
- * tensile rupture energy
- * burst
- * tear
- * scattering coefficient

SMALL-STRAIN THEORIES OF ISOTROPIC SOLIDS (VAN DEN AKKER)

Structural Theories (Cox, Page and Seth, Perkins and Mark)

paper = network of structural elements (fibers)
connected at discrete points (bonds).

PAGE'S STRUCTURAL MODELS

Elastic modulus of the isotropic sheet

$$E_{iso} = \frac{E_f}{3} \left(1 - \frac{W}{L \cdot RBA} \left(\frac{E_f}{2G_f} \right)^{\frac{1}{2}} \right)$$

$$RBA = (SL_u - SL) / SL_u$$

MODIFIED PAGE MODEL

Including kink, curl and microcompressions,

$$E_{iso} = \frac{E_f}{3} \left(1 - \frac{W(n_f+1)}{L \cdot RBA} \left(\frac{E_f}{2G_f} \right)^{\frac{1}{2}} \right)$$

n_f = number of crimps

MOLECULAR THEORIES (HYDROGEN-BOND THEORY OF NISSAN)

paper = continuum of intermolecular
covalent and hydrogen bonds

Temperature Dependence (Nissan and Batten)

$$\frac{d \ln(E)}{d T} = -2.4 \times 10^{-3} \text{ deg}^{-1}$$

MOLECULAR THEORIES

Moisture and humidity sensitivity (Nissan, Battan)

$$\ln(E/E_0) = -h \quad 0 < h < 0.045$$

$$\ln(E/E_0) = -6.407 \cdot h + 0.2433 \quad h > 0.045$$

$h = 0.08$ corresponds to 50% humidity

COMBINATION OF PERCOLATION AND MOLECULAR THEORIES (Nissan and Battan)

$$E_{iso} = 0 \quad d < 126.6 \text{ kg/m}^3$$

$$E_{iso} = \frac{\gamma \cdot 0.4511 \cdot d \cdot (d - 126.6)^{0.35} \hat{E}}{\hat{d}^{1.35}}$$

$$126.6 < d < 357.6$$

$$E_{iso} = \gamma \hat{E} \left(\frac{d}{\hat{d}}\right)^2 \quad d > 357.6$$

CLARK'S ANALYSIS OF PAGE EQUATION

$$RBA = k^2 d \cdot W / (t_f + W)$$

Suggests relation between RBA and d

BOND STRENGTH

- * Proportional to shear modulus G_f
- * G_f proportional to fiber tensile strength, Z (Helle)

$$G_f = k \cdot Z_f = k \cdot Z$$

$$k = .005 \text{ to } .01$$

- * k decreases with moisture

UNTREATED FIBER PROPERTIES

- * Modulus
- * Tensile strength
- * Density
- * Average length
- * Average diameter
- * Composition
- * Fibril angle
- * Bending modulus
- * Cell wall thickness

FACTORS INFLUENCING FIBER PROPERTIES

- * Species, Growth Pattern
- * Pulping
- * Bleaching
- * Moisture
- * Refining

PULPING PROCESS

- * Yield
- * Kappa
- * Removal of hemicellulose
- * Zero span tensile strength
- * Bending stiffness
- * Coarseness
- * Defects

EFFECT OF YIELD

Direct:

- * fiber density and stiffness
- * radial distribution of hemicelluloses and lignin

Indirect:

- * external fibrillation (CSF)
- * internal delamination
 - bending modulus
 - swelling
 - wet compressibility

FIBER LENGTH AND WIDTH DISTRIBUTIONS

- * Species dependent
- * Normal or log-normal
- * Not markedly changed in the pulping step

REFINING

- * Increases fiber external surface (reduces CSF)
- * Increases internal delamination
 - flexibility, conformability
- * Reduces fiber length slightly
- * Breaks up fiber bundles (reduces particle width)

REFINING VARIABLES

- * Net specific power (chemical pulps)
- * Net specific edge load (high yield pulps)
- * Consistency
- * Fiber strength
- * Bending modulus \propto to cell wall thickness
- * Hemicellulose content (surface)
- * Temperature

BOND AREA

- * Measured by relative bonded area
- * Proportional to apparent sheet density
- * Affected by moisture and hemicellulose
- * Proportional to external and internal surface area

BEATING AND REFINING

* Chemical Pulps

- uniform surface area
- internal delamination
- fewer fines

* High Yield Pulps

- nonuniform surface area
- more fines

REFINING

Length and Width Distributions

* High Yield Pulps

- Yan kinetic models

* Chemical Pulps

- Yan or Kane models

SURFACE AREA DEVELOPMENT

* High Yield Pulps

* K-factor Model

NET SPECIFIC POWER

NSP = f(throughput, rpm, consistency, gap) (Miller).
number of passes a drawback

FREENESS

Measure of external surface area - S

$S = a \cdot \ln(\text{CSF}) + b$ high yield pulps (Stationwala)

$S = a \cdot \text{CSF} + b$ chemical pulps (Yan)

$S = f(\text{filtration resistance})$ independent of yield (Doshi)

WET COMPRESSIBILITY

$$\Delta d = M \cdot p^N$$

- * N increases with decreasing CSF (Cowan)
- * M increases with decreasing yield.
- * M increases with moisture

DRYING

- * Surface tension forces increase as
 - inter-fiber water removed (Campbell effect)
 - surface area increases
- * Network forces increase as
 - intra-fiber moisture removed
 - fiber diameter decreases

ANISOTROPY

- * Orientation and Stretch
 - similar
 - complementary
- * Influence
 - stress distribution
 - anisotropy ratios

EFFECT ON PROPERTIES (SETTERHOLM, KUENZI, PARSONS)

- * Orientation and Stretch Interact
 - MD tensile index and modulus increase and pass through a maximum
 - Maxima increase with increasing orientation angle
 - Maxima occur at approximately 1% stretch
 - Main effect appears to be on MD/CD ratio of elastic modulus and breaking length

FORMATION

- * Variation in density (d_{CV})
- * Results from basis weight and thickness variations
- * One cause of variations in sheet properties

FORMATION (GRABER AND GOTTSCHING 1979)

- * Optimal (minimum) values near machine conditions
- * Minimal for jet/wire ratio of 1.08
- * CD CV values were generally less than MD CV values
- * Small influence of machine speed on MD CV in basis weight and thickness
- * CD CV decreases with increasing speed
- * Lower for the high turbulence headbox

SHAKE

- * Frequency and amplitude influence
 - fiber orientation in the machine direction
 - density CV

DEWATERING, DRAINAGE AND RETENTION

* Main effects

- fines retention
- formation

Currently modeled with mixers and splitters (clarifiers)

DIMENSIONAL STABILITY (MILLER, 1977)

* Shrinkage depends on

- refining extent (surface area)
- rheological stress history

POROSITY

* Related to

- pore size
- sheet density and basis weight

* Pore size decreases with

- increasing basis weight (Van den Akker)
- increasing sheet density at any given basis weight

OPTICAL PROPERTIES

Kubelka-Munk theory of light transmission

$$R_{inf} = 1 + (k/SL) - ((k/SL)^2 + 2*(k/SL))^{1/2}$$

brightness = R_{inf} at 457 nm.

k (absorptivity) depends on species, pulping and bleaching

SL (scattering) depends on density

PROPOSED PERFORMANCE ATTRIBUTE MODELS

DENSITY MODEL

Slurry:

$$d = (1-e)*d_f + e*d_v$$

Dry Network

$$d = (1-e)*d_f$$

FIBER DENSITY

$$d_f = (1-e_f)*d_s + e_f*d_v$$

SOLID DENSITY

$$1/d_s = x_c/d_c + x_l/d_l + (1-x_c-x_l)/d_h$$

Saturated fiber

$$d_f \approx 1$$

Collapsed dry fiber

$$d_f = d_s*(1-e_f)$$

Upper limit

$$d_f = d_c \approx 1.54 \text{ g/cc}$$

SHEET DENSITY IN TERMS OF RBA

$$RBA = k*W*d/(t_f + W)$$

$$d = d_f*RBA*(t_f+W)/W$$

EXPECT d TO DECREASE WITH FIBER THICKNESS, t_f

$$d = d_f \cdot \text{RBA} = d_f \cdot (1-e)$$

$$\text{RBA} = 1-e$$

RBA MODEL

$$\text{RBA} = f(S_b)$$

After refining, prior to wet pressing and drying

$$S_b = c \cdot S_h$$

S_h = internal and external surface from refining

$$c = f(\text{polarity, consistency})$$

$$\text{RBA} = S_b / (k_1 + S_b)$$

$$d = d_f \cdot S_b / (k_1 + S_b)$$

LIMITING CONDITIONS

$$d = d_u \text{ when } S_b = S_u \text{ (unbonded sheet)}$$

$$k_1 = S_u \cdot (d_f / d_u - 1)$$

d approaches d_f (unity) as S_b becomes large

DENSITY MODEL

$$d = \frac{d_f S_b}{(S_u(\frac{d_f}{d_u} - 1) + S_b)}$$

$$d_u = .13 \text{ (Nissan) to } .3 \text{ (Malmberg)}$$

$$d_u \propto \frac{\gamma/L}{E_f CWT^2}$$

$$S_u = c_u * S_h + c_0 \text{ (relatively independent of refining)}$$

$$c_u = c(\text{butyl alcohol or low consistency})$$

SURFACE AREA MODEL

K-factor model used for mechanical pulping

$$S_h = 1 - \sum (X_i * \ln(L_i/L_a)) / K$$

$$K = K_0 * e^{(k_2 * NSP)}$$

$$k_2 = f(NSP, \text{Consistency}, K_0)$$

MORE GENERAL K-FACTOR MODEL

$$k_2 = f(NSP, \text{refining consistency, composition, temperature, CWT, fiber strength, } E_f)$$

S_h driven downward during drying

REFINER MODEL

Kinetic models (Yan) used for mechanical pulping

$$L = A_1 + (L_{in} - A_1/A_2)\exp(-A_1*ZP)$$

$$\sigma L = A_1 - A_2/L$$

$$ZP = 10^{(NSP - A_p)/B_p}$$

Width parameters similar

FREENESS MODEL

$$S_h = S_1 - S_2*\ln(CSF) \text{ (mechanical pulp)}$$

$$S_h = S_1 - S_2*CSF \text{ (chemical pulp)}$$

FIBER FRACTIONATION

Current HYFRAC models

Total flow split, L and W

Conservation of S_h

No separation on fiber density

FIBER MIXING

- * Mixing rules
- * Conservation of S_h
- * Weight-averaging

WET PRESSING

We observe

$$d = d_i + M \cdot P^N$$

This results from

$$S_b = S_{b0} \cdot (1 + M \cdot P^N)$$

$$S_{b0} = C \cdot S_h \quad (\text{1st press nip})$$

$$M = M_1 + M_2 \cdot Y$$

$$N = N_1 + N_2 \cdot S_h$$

ELASTIC MODULUS (MALMBERG, PARSONS)

$$RBA = (SL_u - SL) / SL_u$$

$$SL_u - SL = k_4 \cdot (d - d_u)$$

$$k_4 \text{ is approximately } SL_u$$

$$RBA = k_4 (d - d_u)$$

Normalization

$$k_4 = 1 - d_u$$

$$RBA = (d - d_u) / (1 - d_u)$$

ISOTROPIC ELASTIC MODULUS

$$E_{iso} = \frac{E_f}{3} \left[1 - \frac{W(1-d_u)}{L(d-d_u)} \left(\frac{E_f}{2G_f} \right)^{\frac{1}{2}} \right]$$

$$d > d_u + \frac{W(1-d_u)}{L} \left(\frac{E_f}{2G_f} \right)^{\frac{1}{2}}$$

Otherwise

$$E_{iso} = 0$$

FIBER GEOMETRY

$$t_f = 2 * CWT$$

$$CWT = f(\text{species})$$

$$P = 2 * (t_f + W)$$

$$A = W * t_f$$

$$P_r = \pi * D_f$$

$$P = P_r$$

$$W_r = P_r / 2 - 2 * CWT$$

BOND STRENGTH

Bond strength \propto shear modulus

Shear modulus \propto intrinsic fiber strength

$$G_f = c * Z_f = c' * Z$$

$$c' = f(\text{moisture})$$

FIBER MODULUS

Strength decrease with removal of cellulose

$$Z = Z_{fu}*(1 - k*DC)$$

$$E_f = E_{fu}*(1 - k'*DC)$$

Z_{fu} , E_{fu} untreated fibers

TEMPERATURE DEPENDENCE (NISSAN AND BATTEN)

$$E_{iso}^T = E_{ref}*e^{k*(T-T_{ref})}$$

$$k = -2.4 \times 10^{-3}$$

$$T_{ref} = 25^{\circ}\text{C}$$

$E_{ref} = E_{iso}$ at 25°C , 50% humidity (Page Model)

MOISTURE SENSITIVITY (NISSAN, BATTAN)

$$E_{iso}^h = E_{iso}^T e^{-(h-0.08)} \quad 0 < h < 0.045$$

$$E_{iso}^h = E_{iso}^T e^{-6.407(h-.0424)+0.2433} \quad h > 0.045$$

$h = 0.08$ corresponds to 50% humidity

SHEET ANISOTROPY

Geometric Mean of MD and CD

$$E_{iso} = (E_{MD} \cdot E_{CD})^{1/2}$$

$$E_{MD} = E_{iso} \cdot R^{1/2}$$

$$R = E_{MD}/E_{CD}$$

EFFECT OF ORIENTATION

$$OR = \cotan(\theta)$$

$$\ln(E_{MD}) = a \cdot \ln(OR) + b$$

a and b functions of s and pulp type

Interaction between OR and s

$$R = E_{MD}/E_{CD} = c \cdot OR \cdot (1 + k \cdot (s - s_0))$$

c approximately 1.09

k approximately -.0054

s₀ about -12%.

FORMATION (GRABER, GOTTSCHING)

$$d_{CV} = A \cdot MS + B \cdot MS^2 + C \cdot JWR + D \cdot JWR^2 + E \cdot CO + F \cdot CO^2$$

$$+ G \cdot (SA \cdot SF) + H \cdot (SA \cdot SF)^2$$

MS = machine speed

JWR = jet-wire ratio

CO = head box consistency

SA = shake amplitude

SF = shake frequency

EFFECT OF FORMATION ON BURST

$$B = f(E_b) * t = f(E * t) * t = f\left(\frac{E}{d}\right)$$

$$B = k\left(\frac{E^3}{d}\right)\frac{1}{d}$$

$$d_{\max} = d_{\text{mean}}(1 + d_{\text{cv}})$$

$$d_{\min} = d_{\text{mean}}(1 - d_{\text{cv}})$$

$$B_{\max} = k * E_{\max}^3 / d_{\max}^2$$

$$E_{\max} = E_{\text{iso}}, E_{\text{MD}} \text{ or } E_{\text{CD}} \text{ at } d_{\max}$$

BRIGHTNESS

$$SL \propto d - d_u$$

$$C_k \propto X_1$$

X_1 changed during bleaching

Brightness from Kubelka-Munk Equation

MECHANICAL PROPERTIES

* Power-law Models

$$\text{PROP} = k * (E/d)^m$$

- bending modulus
- breaking length
- elongation
- tensile rupture energy

$$\text{PROP} = k * E^m / d^n$$

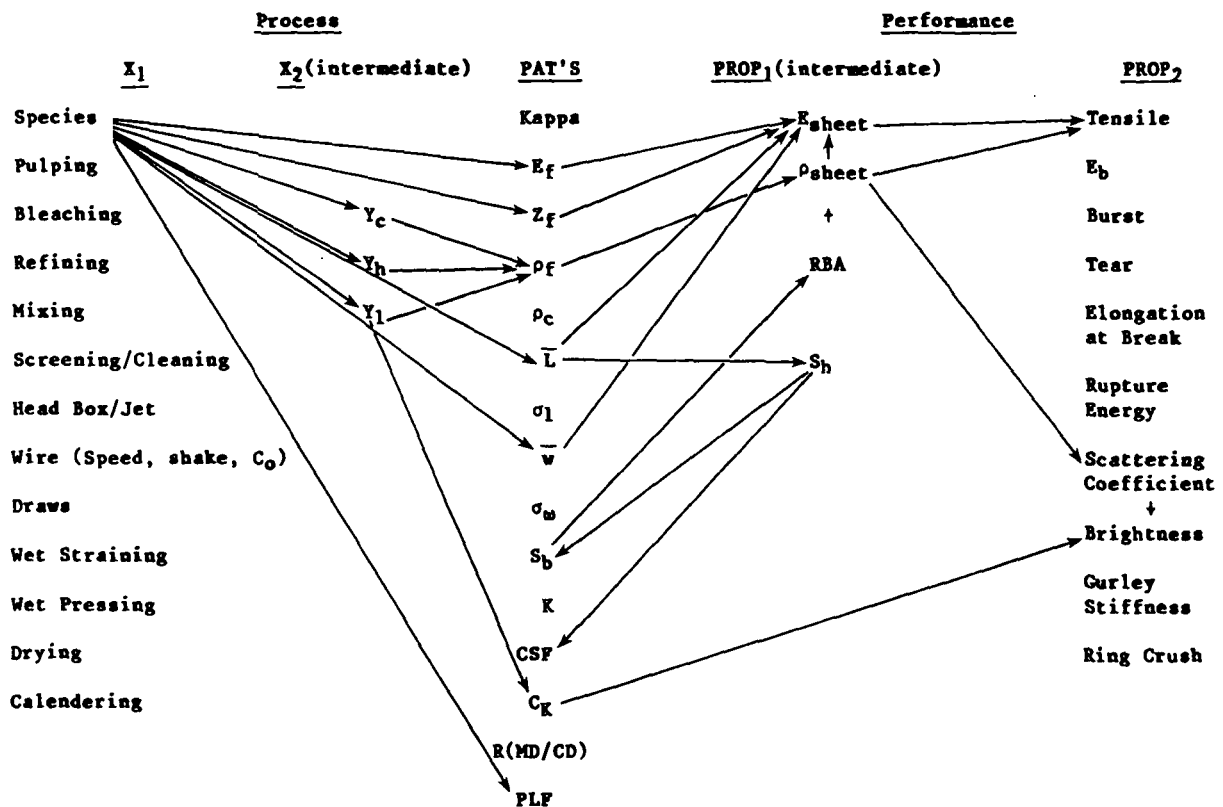
- burst factor
- tear factor

$$E = E_{\text{iso}}, E_{\text{MD}}, E_{\text{CD}}$$

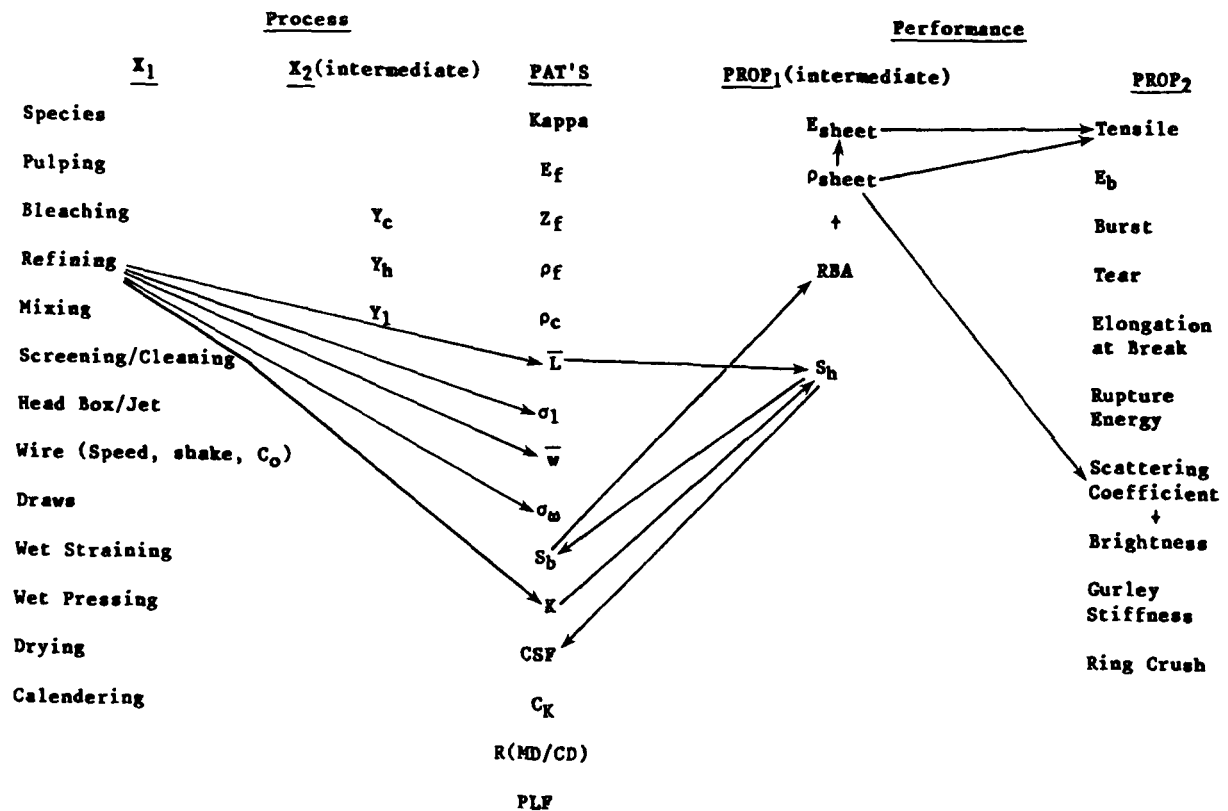
OTHER MECHANICAL PROPERTIES (KELLOGG)

- * Compressive properties (i.e. Ring Crush)
- * Converting properties (printability)
- * Optical and surface properties (i.e. opacity, porosity)

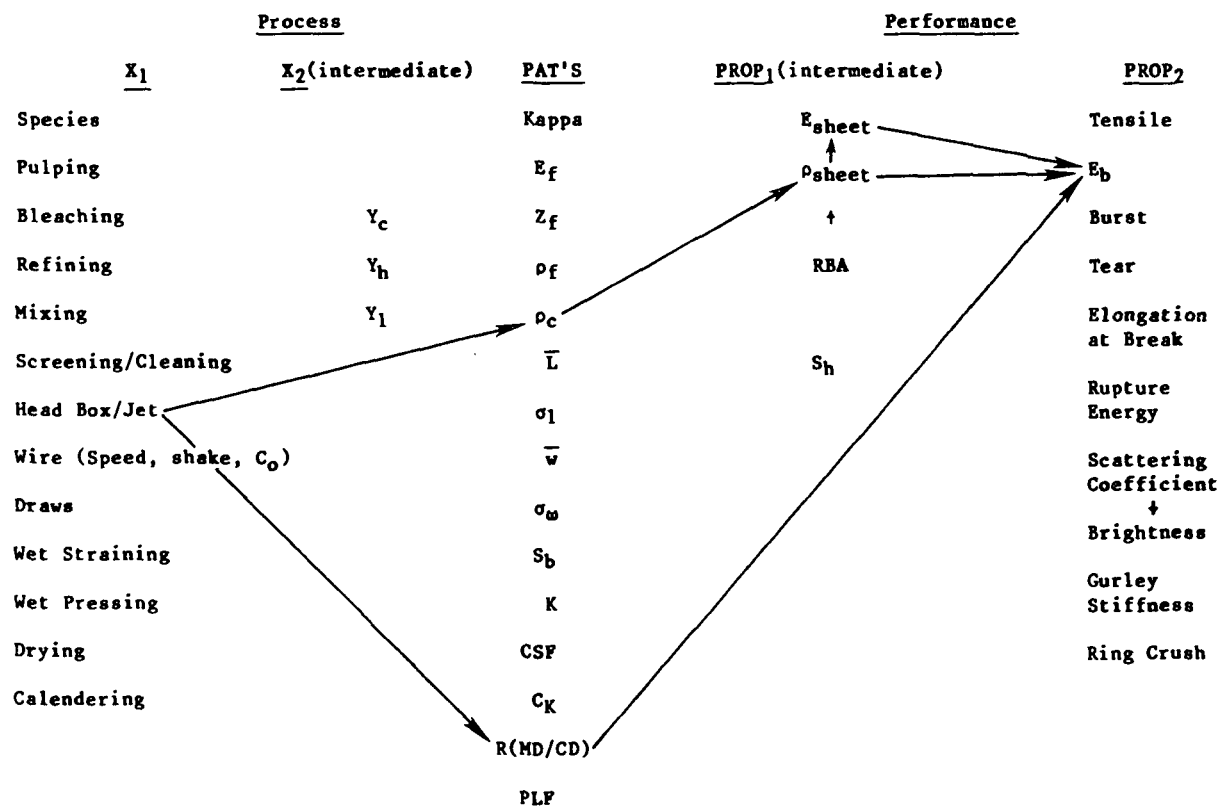
Relationships Between Process Variables, Performance Attributes and End-Use Performance



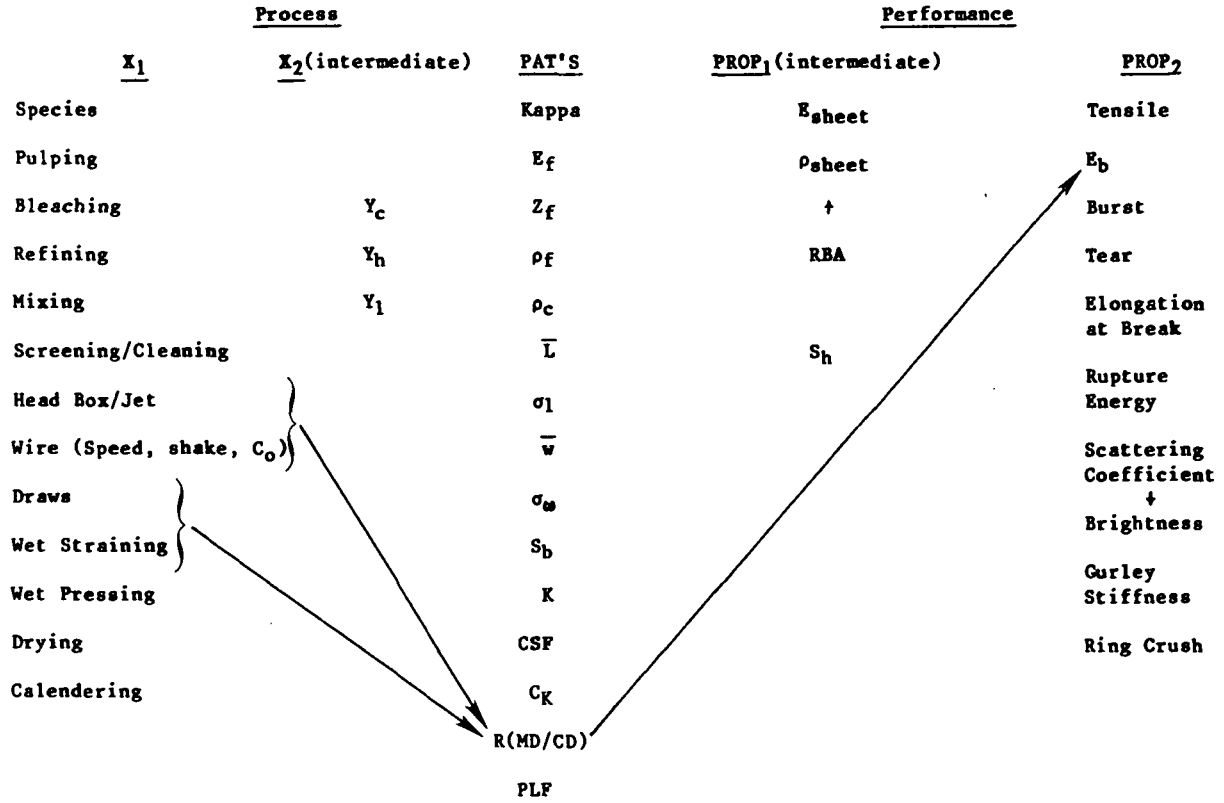
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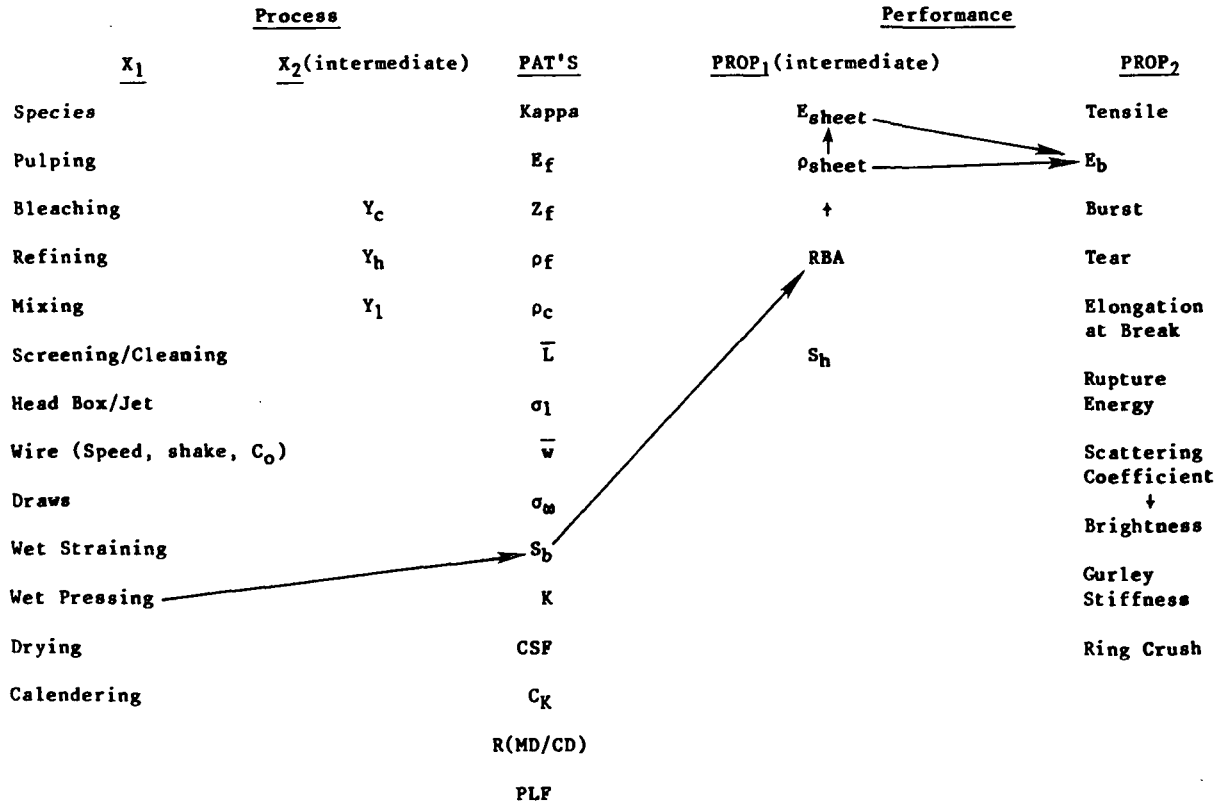
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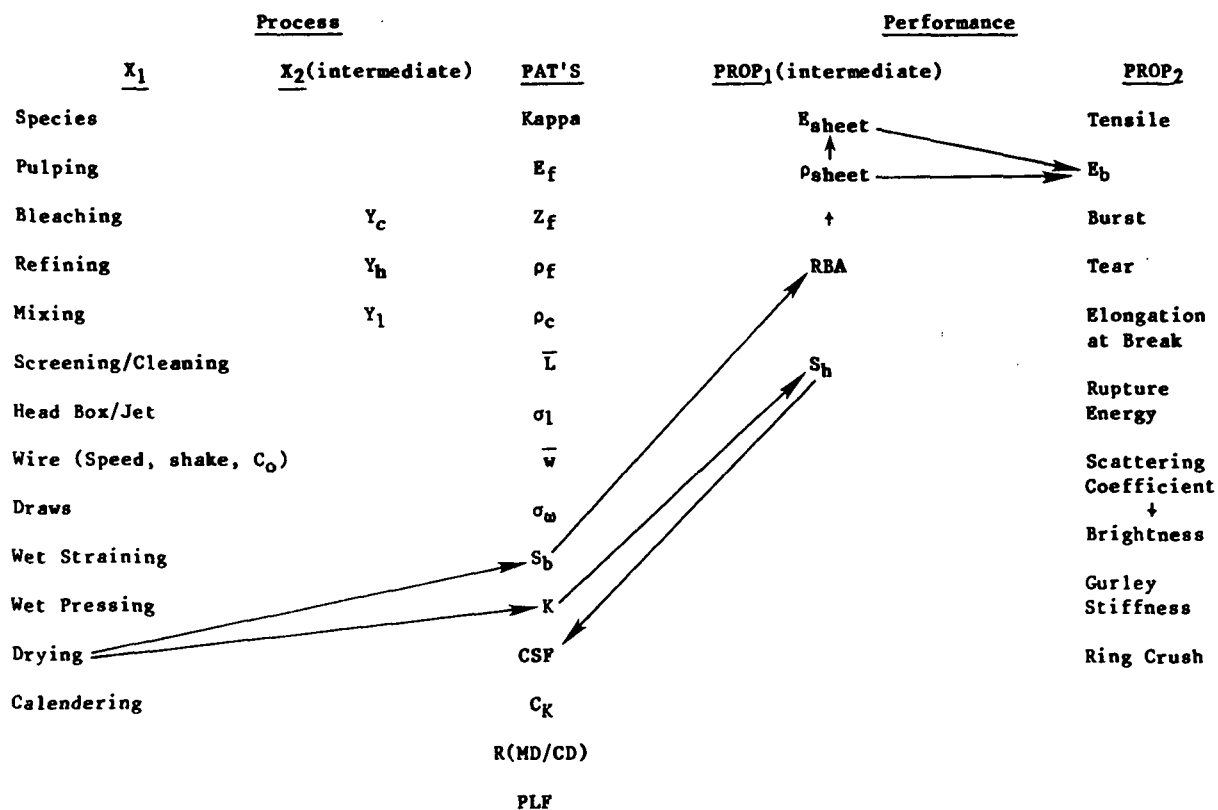
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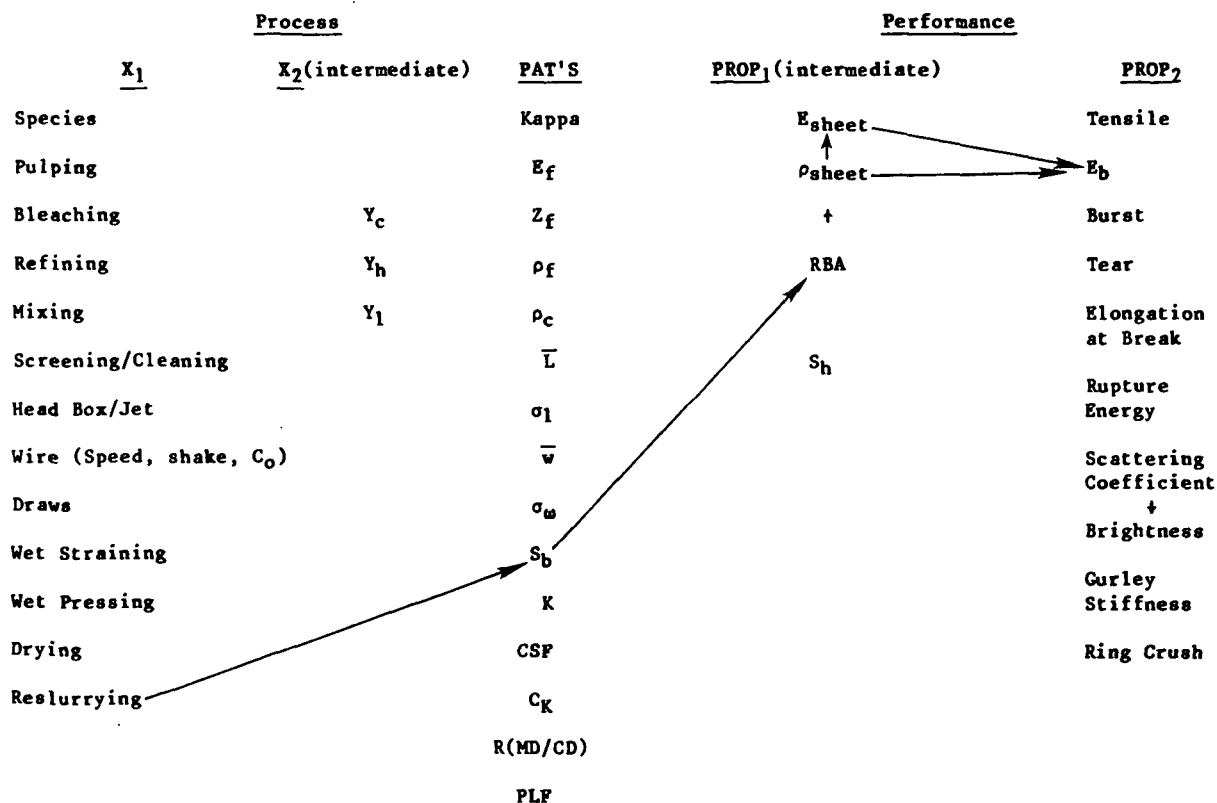
Relationships Between Process Variables, Performance Attributes and End-Use Performance



Relationships Between Process Variables, Performance Attributes and End-Use Performance



Relationships Between Process Variables, Performance Attributes and End-Use Performance



MODEL VALIDATION

- * Develop Data Base
- * Nonlinear programming outside MAPPS
- * Integrate into MAPPS
- * Test against mill data